Computational properties of three-term recurrence relations for Kummer functions

Alfredo Deaño [a] Javier Segura [b] Nico M. Temme [c]

[a] *Department of Applied Mathematics and Theoretical Physics, Univ. of Cambridge, Wilberforce Road, Cambridge CB3 0WA, UK*

[b] *Departamento de Matemáticas, Estadística y Computación, Univ. de Cantabria, 39005 Santander, Spain*

[c] *CWI, P.O. Box 94079, 1090 GB Amsterdam, The Netherlands*

Dedicated to Jesús S. Dehesa on the occasion of his 60th birthday

Abstract

Several three-term recurrence relations for confluent hypergeometric functions are analyzed from a numerical point of view. Minimal and dominant solutions for complex values of the variable z are given, derived from asymptotic estimates of Whittaker functions with large parameters. The Laguerre polynomials and the regular Coulomb wave functions are studied as particular cases, with numerical examples of their computation.

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1 Introduction

Three-term recurrence relations (TTRR) are well-known identities in the theory of hypergeometric functions, and their numerical properties for computational purposes have been studied in several references, for instance in [5] and [9]. More recently, recursions for Gauss hypergeometric functions have been

Email addresses: ad495@cam.ac.uk (Alfredo Deaño), javier.segura@unican.es (Javier Segura), nicot@cwi.nl (Nico M. Temme).

examined in detail in [6, Ch. 4], and several TTRR for confluent hypergeometric functions have been analyzed in [3].

In all cases, the stability of these recurrence relations is crucial for a reliable numerical implementation, and in this sense the key idea is the notion of minimal and dominant solutions of the recursion. Given a three-term recurrence relation of the form:

$$y_{n+1}(z) + b_n y_n(z) + a_n y_{n-1}(z) = 0, \tag{1}$$

where n is an integer parameter, a solution $f_n(z)$ is said to be minimal (or recessive) when $n \to +\infty$ (forward direction) if

$$\lim_{n\to+\infty} \frac{f_n(z)}{g_n(z)} = 0, \tag{2}$$

for any other solution $g_n(z)$ of (1) that is linearly independent of $f_n(z)$ (provided that this limit exists). The solution $g_n(z)$ is said to be dominant. We point out that the minimal and dominant solutions depend on the direction in which the TTRR is analyzed, and if we use (1) in the backward direction (that is, with $n \to -\infty$), a different pair of dominant and minimal solutions may arise.

Whenever a three term recursion admits a minimal solution $f_n(z)$, this solution is distinguished both in the sense that it is needed in order to construct a numerically satisfactory pair of solutions of (1), see [6], and because of the problems that arise in its computation when (1) is used in the forward direction (increasing n).

These difficulties stem from the fact that a generic solution of (1), say $y_n(z) = Af_n(z) + Bg_n(z)$, where A and B do not depend on n, behaves like a dominant solution whenever $B \neq 0$. Since the condition $B = 0$ is usually not satisfied in numerical computations (if only because of rounding errors), the numerical solution $y_n(z)$ is dominant, and the error with respect to $f_n(z)$ becomes unacceptably large when we use the recursion in the forward direction. As a result of this, the detection and identification of minimal solutions is of paramount importance prior to the use of the three-term recursions for computations.

We remark that when a solution $f_n(z)$ is minimal in the forward direction, the recursion may be very useful for computing $f_n(z)$ in the backward direction. Efficient schemes, such as the Miller algorithm, are available in that case, and sometimes exact starting values are not strictly needed. We refer the reader to [6, §4.6] for more information and computational details. In particular, it is of importance to note that the continued fraction associated to the recursion (1), that is:

$$\frac{y_n}{y_{n-1}} = \frac{-a_n}{b_n+} \frac{-a_{n+1}}{b_{n+1}+} \frac{-a_{n+2}}{b_{n+2}+} \cdots$$

exhibits good numerical properties precisely for the computation of the ratio of minimal solutions f_n/f_{n-1}.

We consider recursions for the Kummer functions

$$ {}_1F_1(a+\epsilon_1 n; c+\epsilon_2 n; z), \qquad U(a+\epsilon_1 n, c+\epsilon_2 n, z), \tag{3} $$

where ϵ_i are integers ($\epsilon_1 = \epsilon_2 = 0$ excluded). Naturally, the choice of ϵ_1 and ϵ_2 will produce different directions of recursion. We recall the notation used in [3]. For example, when $\epsilon_1 = 1$ and $\epsilon_2 = 0$, the recursion is denoted by $(+\,, 0)$, when $\epsilon_1 = 2$ and $\epsilon_2 = -1$, it is denoted by $(2+\,, -)$.

In [3] the minimal solutions of the Kummer recursions were obtained by means of Perron's theorem combined with uniform asymptotic expansions of Whittaker functions for large values of the parameters κ and μ, see [4] and [7]. These estimations, together with connection formulas available for the solutions of Kummer differential equation, suffice to give minimal and dominant solutions for these recursions.

In this paper we will concentrate on two examples as an illustration of these results: Laguerre polynomials, where we will use the recursions $(-, 0)$ and $(-, +)$ (with opposite behavior with respect to the computation of these polynomials), and Coulomb wave functions. This last example, already considered in [5], will be obtained as a particular case of the more general $(+, 2+)$ recursion for Kummer functions; this recursion is analyzed from the asymptotic estimates derived in [7].

2 Laguerre polynomials

Laguerre polynomials can be written as confluent hypergeometric functions, the first parameter being a negative integer, see [1],[9, p. 190]:

$$ L_n^{(\alpha)}(z) = \frac{(-1)^n}{n!}\, U(-n, \alpha+1, z) = \binom{n+\alpha}{n} {}_1F_1(-n; \alpha+1; z), \tag{4} $$

where n is the degree of the polynomial.

2.1 Recursion and asymptotic analysis

The recursion (1) for increasing n corresponds to the $(-,0)$ case in Kummer notation. This recursion has the following coefficients:

$$a_n = \frac{n-a}{c-a+n}, \quad b_n = \frac{2a-2n-c+z}{c-a+n}, \tag{5}$$

with the asymptotic behavior:

$$a_n \sim 1, \quad b_n \sim -2, \quad n \to \infty. \tag{6}$$

It follows from Perron's theorem (see [9, Theorem 13.1, Case 2] and [6, §4.3] that

$$\limsup_{n\to\infty} |y_n(z)| = 1, \tag{7}$$

for each non-trivial solution of the recursion.

Four different solutions are

$$\begin{aligned} y_n^{(1)}(z) &= {}_1F_1(a-n;c;z), \\ y_n^{(2)}(z) &= \frac{(-1)^n}{\Gamma(c-a+n)}\, U(a-n,c,z), \\ y_n^{(3\pm)}(z) &= \Gamma(1-a+n)\, U(c-a+n,c,ze^{\pm\pi i}). \end{aligned} \tag{8}$$

In the Laguerre case $a=0$ and $c=\alpha+1$, and it is clear from (4) that the first and second solutions are not linearly independent. For this reason, we will take the following set:

$$\begin{aligned} y_n^{(1)}(z) &= \frac{\Gamma(n+\alpha+1)}{\Gamma(n+1)\Gamma(\alpha+1)}\ {}_1F_1(-n;\alpha+1;z), \\ y_n^{(2\pm)}(z) &= \frac{\Gamma(n+\alpha+1)}{\Gamma(\alpha+1)}\, U(n+\alpha+1,\alpha+1,ze^{\pm\pi i}). \end{aligned} \tag{9}$$

The information given by Perron's theorem in (7) is not sufficient to identify the minimal and dominant solutions, and we need details on the asymptotic behavior of the Kummer functions for large values of the parameters. In the literature this information is available for the Whittaker functions (see [1,

p. 505]):

$$M_{\kappa,\mu}(z) = e^{-z/2} z^{1/2+\mu}\, {}_1F_1(\tfrac{1}{2}+\mu-\kappa; 1+2\mu; z),$$
$$W_{\kappa,\mu}(z) = e^{-z/2} z^{1/2+\mu}\, U(\tfrac{1}{2}+\mu-\kappa, 1+2\mu, z). \tag{10}$$

For the solutions of the $(-,0)$ recursion, with parameters $a-n$ and c, the Whittaker parameters are:

$$\kappa = \tfrac{1}{2}(c-2a+2n) = \tfrac{1}{2}(2n+\alpha+1), \qquad \mu = \tfrac{1}{2}(c-1) = \tfrac{1}{2}\alpha, \tag{11}$$

and therefore, the asymptotic behavior for $n \to +\infty$ corresponds to the large κ behavior (and fixed μ) of the Whittaker functions. This situation can be analyzed by using the estimates given in [4, Eqns. 6.7-6.10], see also [3].

Let us begin with the analysis of the solutions $y_n^{(2\pm)}(z)$ in formula (9). The information about the solution $y_n^{(1)}(z)$ can then be obtained by using the following connection formula (see [8, p. 28]):

$$M_{\kappa,\mu}(z) = \frac{1}{2\pi}\Gamma(2\mu+1)\Gamma(\kappa-\mu+\tfrac{1}{2})\left[e^{-\mu\pi i} W_{-\kappa,\mu}(ze^{-\pi i}) + e^{\mu\pi i} W_{-\kappa,\mu}(ze^{\pi i})\right]. \tag{12}$$

The solutions $y_n^{(2\pm)}(z)$ can be written in terms of the Whittaker functions $W_{-\kappa,\mu}(ze^{\pm\pi i})$, where κ and μ are given by (11). As stated in [3], the main contributions for large κ are given in terms of Hankel functions:

$$y_{\kappa,\mu}^{(2-)}(z) = \Gamma(\kappa+\mu+\tfrac{1}{2})\, W_{-\kappa,\mu}(ze^{-\pi i}) \sim F_{\kappa,\mu}(z) H_{2\mu}^{(1)}(2\sqrt{\kappa z}), \tag{13}$$

$$y_{\kappa,\mu}^{(2+)}(z) = \Gamma(\kappa+\mu+\tfrac{1}{2})\, W_{-\kappa,\mu}(ze^{\pi i}) \sim e^{-2\mu\pi i} F_{\kappa,\mu}(z) H_{2\mu}^{(2)}(2\sqrt{\kappa z}), \tag{14}$$

where

$$F_{\kappa,\mu}(z) \sim \pi\sqrt{z}\; e^{\mu\pi i}\kappa^{\mu}, \qquad \kappa \to \infty. \tag{15}$$

and the principal branches of the square roots are taken, which are real on the positive real axis.

The behavior of the Hankel functions for large complex values of the argument is well known, see for instance [1, Eqns. 9.2.3 and 9.2.4]. Namely:

$$H_\nu^{(1)}(w) \sim \sqrt{\frac{2}{\pi w}}\; e^{i(w-\frac{1}{2}\nu\pi-\frac{1}{4}\pi)}, \quad -\pi < \operatorname{ph} w < 2\pi, \tag{16}$$

$$H_\nu^{(2)}(w) \sim \sqrt{\frac{2}{\pi w}}\; e^{-i(w-\frac{1}{2}\nu\pi-\frac{1}{4}\pi)}, \quad -2\pi < \operatorname{ph} w < \pi, \tag{17}$$

as $w \to \infty$. Depending on the location of w in the complex plane, the Hankel functions can be exponentially large, exponentially small or they can have oscillatory real and imaginary parts. Taking into account (12), it is clear that the minimal solution will be the one that exhibits an exponentially small behavior (if any). This leads to the following result:

- When $\Im(z) < 0$ then $H_{2\mu}^{(1)}(2\sqrt{\kappa z})$ is exponentially small, and $y_n^{(2-)}(z)$ is the minimal solution, whereas $y_n^{(2+)}(z)$ and $y_n^{(1)}(z)$ are dominant.
- When $\Im(z) > 0$ then $H_{2\mu}^{(2)}(2\sqrt{\kappa z})$ is exponentially small, and $y_n^{(2+)}(z)$ is the minimal solution, and $y_n^{(2-)}(z)$ and $y_n^{(1)}(z)$ are dominant. This behavior holds when z is real and negative, taking the principal argument $\operatorname{ph} z = \pi$.
- When z is real and positive (on the classical interval of orthogonality), the real and imaginary parts of both Hankel functions oscillate, and there are no minimal/dominant solutions.

In any of these cases, for bounded values of z in $|\operatorname{ph} z| < \pi$, the Laguerre polynomials are either dominant solutions or oscillatory when all solutions of the recurrence show a similar behavior. Therefore, when using t he $(-, 0)$ recursion there are no stability problems arising from bad conditioning, and only round-off errors should be taken into consideration for computing Laguerre polynomials.

2.2 Numerical examples

In this section we will use two different recursions to compute Laguerre polynomials, in order to illustrate the importance of knowing whether a solution is minimal or not for a given recursion.

Suppose that we want to compute the Laguerre polynomial $L_N^{(N+\alpha)}(z)$, for given values N and α (N may be large or moderate). One possibility is to start with the initial values $L_0^{(N+\alpha)}(z) = 1$ and $L_1^{(N+\alpha)}(z) = 1 + N + \alpha - z$, and then use the $(-, 0)$ recursion for Kummer functions, modified to take into account the formula (4) and the values $a = 0$, $c = N + \alpha + 1$. The coefficients read:

$$b_n = -\frac{2n + N + \alpha + 1 - z}{n + 1}, \qquad a_n = \frac{n + N + \alpha}{n + 1}, \tag{18}$$

for $n = 1, 2, \ldots, N - 1$.

Another possibility is to begin with $L_0^{(\alpha)}(z) = 1$ and $L_1^{(\alpha+1)}(z) = 2 + \alpha - z$ and

use the $(-,+)$ recursion for Kummer functions. The coefficients are:

$$\begin{aligned} b_n &= \frac{z^3-(\alpha+2)z^2+n(\alpha+3z-5z^2)+n^2(3z+\alpha+1)+n^3}{z(z-n)(n+1)}, \\ a_n &= \frac{(2n+\alpha)(2n+\alpha-1)(z-1-n)}{z(z-n)(n+1)}, \end{aligned} \tag{19}$$

for $n = 1, 2, \ldots, N-1$.

We have analyzed both cases with $\alpha = -0.1$ and two different values of z, programming the recursions in Fortran (fixed double precision) and comparing with the direct computation given by Maple with 30 digits. Figures 1 and 2 show the relative errors between these results for two different values of the variable z.

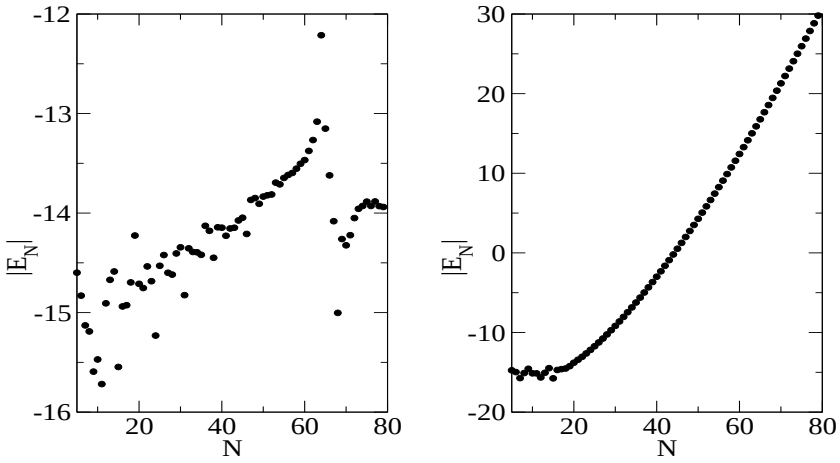

Fig. 1. Relative errors (in $\log_{10}$ scale) in the computation of $L_N^{(N+\alpha)}(z)$, with $z = 2.13$ and $\alpha = -0.1$, using the $(-,0)$ recursion (on the left) and using the $(-,+)$ recursion (on the right).

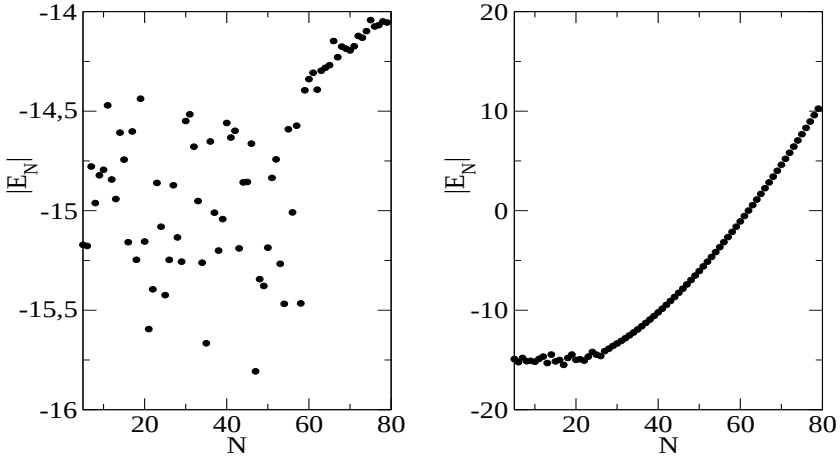

Fig. 2. Same as Figure 1, but with $z = 0.76 + 4.42i$.

As can be seen, the error stays within approximately double precision in the case of the $(-,0)$ recursion, when either all solutions of the recursion are oscillatory (real and positive z) or the Laguerre polynomial is dominant (complex z). On the other hand, when using the $(-,+)$ recursion the Laguerre polynomial is minimal (for details, see [3]), and the instability appears very quickly.

We hasten to remark that this asymptotic analysis is crucial in order to understand the behavior of the recursions, but in an actual computation, that is for finite n, the loss of accuracy due to instability might be acceptable, and it is then indeed possible to use a three-term recurrence relation to compute a minimal solution. Figure 3 shows a similar experiment but with a larger real value of z (and 100 digits in the Maple direct computation). The behavior is the same asymptotically, but the evaluation of the Laguerre polynomial using the $(-,+)$ recursion could be acceptable in standard double precision for $n \leq 120$.

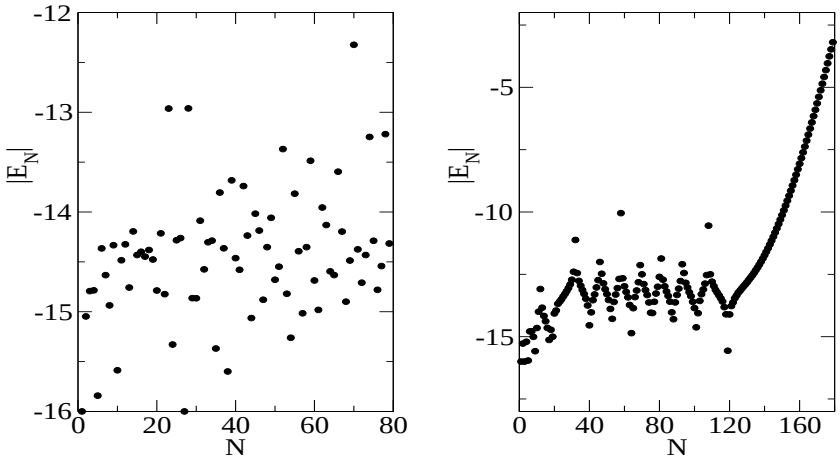

Fig. 3. Relative errors (in $\log_{10}$ scale) in the computation of $L_N^{(N+\alpha)}(z)$, with $z = 21.88$ and $\alpha = -0.1$, using the $(-,0)$ recursion (on the left) and using the $(-,+)$ recursion (on the right).

In some cases, even a reversion in the role of the solutions may take place, in the sense that a dominant solution behaves temporarily like a minimal one and vice versa, and consequently the numerical behavior of the recursion is opposite to what is expected. We refer the reader to [2] for details.

3 Coulomb wave functions

The regular Coulomb wave function is related to the Kummer ${}_1F_1$ function with complex variable and parameters [1, Ch.14]:

$$F_L(\eta, z) = C_L(\eta) z^{L+1} e^{-iz}\ {}_1F_1(L+1-i\eta; 2L+2; 2iz), \tag{20}$$

where

$$C_L(\eta) = \frac{2^L e^{-\pi\eta/2}|\Gamma(L+1+i\eta)|}{\Gamma(2L+2)}, \tag{21}$$

$z > 0$, $\eta \in \mathbb{R}$ and L is a non negative integer.

The recursion with increasing L [1, Eqn. 14.2.3] has been investigated in references [5] and [10], with the result that $F_L(\eta, z)$ is the minimal solution, a dominant one being given by the irregular Coulomb wave function $G_L(\eta, z)$ (see [1, Eqn. 14.1.14] . Taking into account the equation (20), this information can be obtained by using the $(+, 2+)$ recursion for Kummer functions. This recursion has the following coefficients:

$$a_n = -\gamma_n d_n, \qquad b_n = e_n d_n, \tag{22}$$

where

$$e_n = \frac{\gamma_n(\gamma_n - z - 2) + 2\alpha_n z}{\gamma_n - 2}, \qquad d_n = \frac{(\gamma_n^2 - 1)\gamma_n}{\alpha_n(\gamma_n - \alpha_n)z^2}, \tag{23}$$

and we have used the notation $\alpha_n = a + n$, $\gamma_n = c + 2n$ for brevity. For the particular case of Coulomb functions, we have $a = -i\eta$, $c = 0$ and $n = L + 1$, and z should be replaced by $2iz$.

Two solutions of the $(+, 2+)$ recursion are:

$$\begin{aligned} y_n^{(1)}(z) &= {}_1F_1(a+n; c+2n; z), \\ y_n^{(2)}(z) &= \frac{(-1)^n\ \Gamma(c+2n)}{\Gamma(c-a+n)}\ U(a+n; c+2n; z). \end{aligned} \tag{24}$$

The coefficients have the following behavior:

$$a_n \sim -\frac{16n^2}{z^2}, \qquad b_n \sim \frac{16n^2}{z^2}, \qquad n \to \infty, \tag{25}$$

and accordingly, Perron's theorem establishes the existence of two solutions such that:

$$\frac{f_{n+1}(z)}{f_n(z)} \sim 1, \qquad \frac{g_{n+1}(z)}{g_n(z)} \sim -\frac{16n^2}{z^2}, \qquad n \to \infty, \tag{26}$$

the function $f_n(z)$ being minimal.

In terms of the Whittaker functions, the parameters read:

$$\kappa = \tfrac{1}{2}(c - 2a), \qquad \mu = \tfrac{1}{2}(c + 2n - 1), \tag{27}$$

so κ is fixed and μ is large when $n \to \infty$. Olver [7, pp. 260–261 and 368] gives the following asymptotic estimate for large μ cases of the Whittaker

$M-$function:

$$M_{\kappa,\mu}(z) \sim z^{1/2+\mu}, \qquad \mu \to \infty, \tag{28}$$

the estimate being uniformly valid with respect to bounded complex values of κ and z in $|\mathrm{ph}\, z| < \pi$. Bearing in mind the relation between $M_{\kappa,\mu}(z)$ and the Kummer F-function, see (10), it is clear that the Kummer function ${}_1F_1(a+n; c+2n; z)$ corresponds to the minimal solution $f_n(z)$ in (26). Since a and c can be complex without disturbing the limiting behavior, this enlarges the range of values of the Coulomb parameters η and z for which the asymptotic result is valid, in the sense that both can be complex.

We observe that, as particular cases of the Coulomb wave functions, we obtain the standard and modified Bessel functions when $\eta = 0$, see [1, Eqns. 13.6.1 and 13.6.3]:

$$\begin{aligned} J_\nu(z) &= \frac{1}{\Gamma(1+\nu)} e^{-iz} \left(\frac{z}{2}\right)^\nu \ {}_1F_1(\nu+\tfrac{1}{2}; 2\nu+1; 2iz), \\ I_\nu(z) &= \frac{1}{\Gamma(1+\nu)} e^{-z} \left(\frac{z}{2}\right)^\nu \ {}_1F_1(\nu+\tfrac{1}{2}; 2\nu+1; 2z), \end{aligned} \tag{29}$$

and the general result is consistent with the known fact (see [5] or [9]) that these two functions are minimal solutions of the corresponding recursions for increasing order ν, and complex bounded values of z in $|\mathrm{ph}\, z| < \pi$.

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